

23<sup>rd</sup> ICEPP Symposium @ Hakuba, Nagano 20/2/2017

---

# 濃縮ガスによる低速中性子散乱を用いた 未知短距離力探索の手法

---

Koji YAMADA, The Univ. of Tokyo

---

# contents

---

- ❖ 1. Introduction

未知短距離力

- ❖ 1.1 Current limits

- ❖ 2. Scattering law

- ❖ 2.1 Coherent scattering length

濃縮ガスによる  
低速中性子散乱

- ❖ 2.2 Static structure factor

- ❖ 3. Scattering length with new interactions

- ❖ 4. 実験条件の検討

- ❖ 5. Analysis

- ❖ 6. Summary

# 1. Introduction

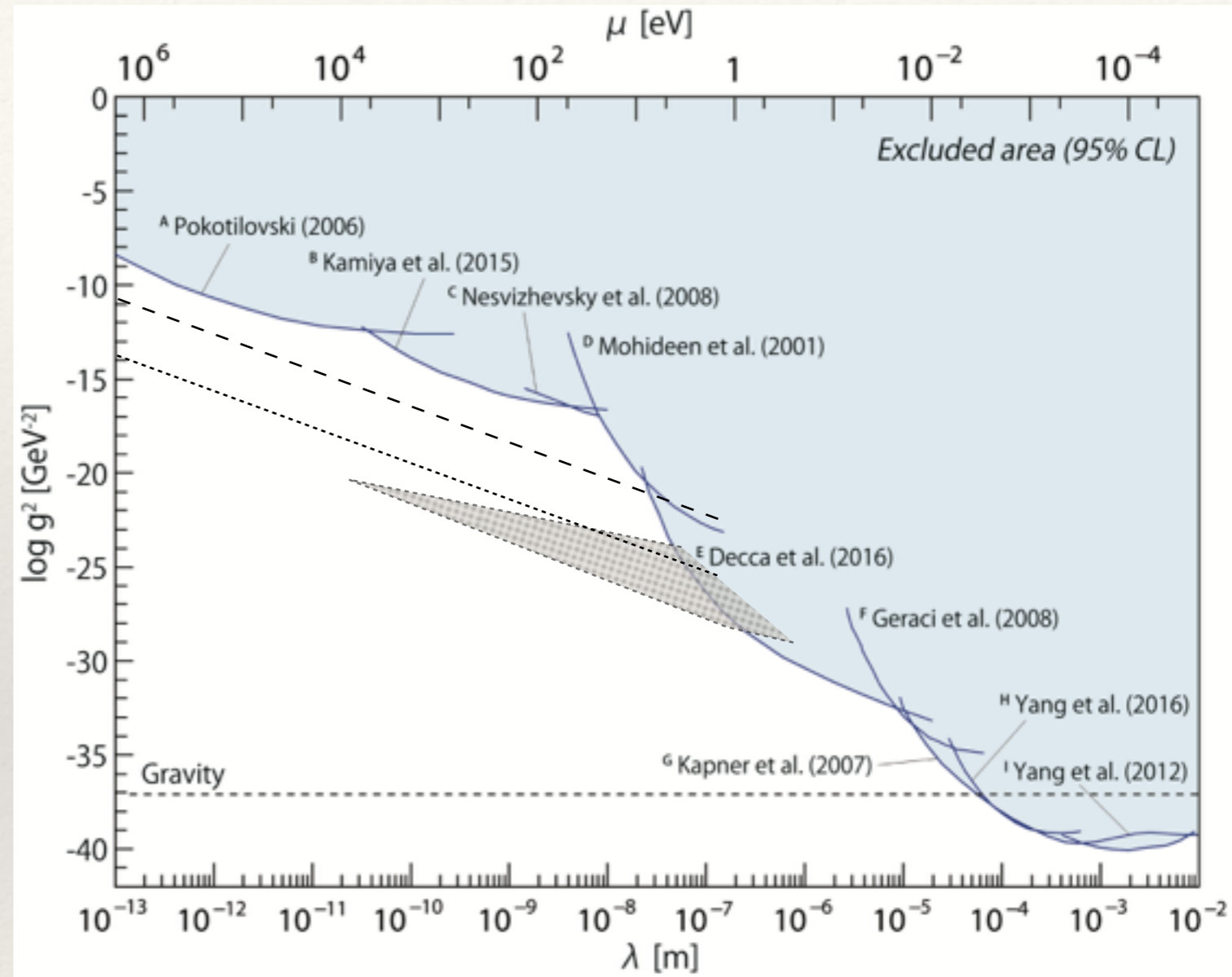
Yukawa-type new interactions

coupling strength

$$V_{\text{new}}(r) = -\frac{1}{4\pi} g^2 Q_1 Q_2 \frac{e^{-\mu r}}{r}$$

coupling charges

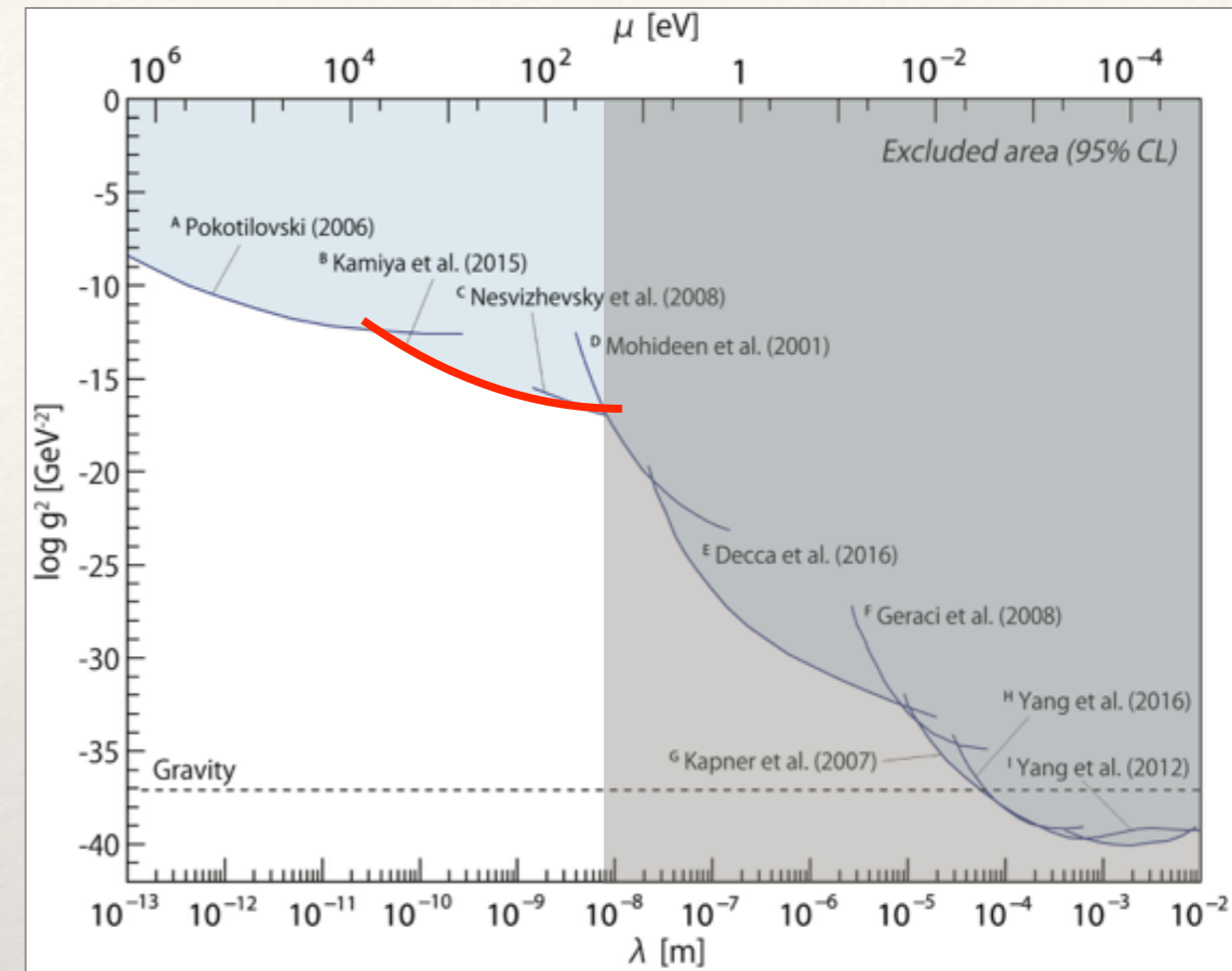
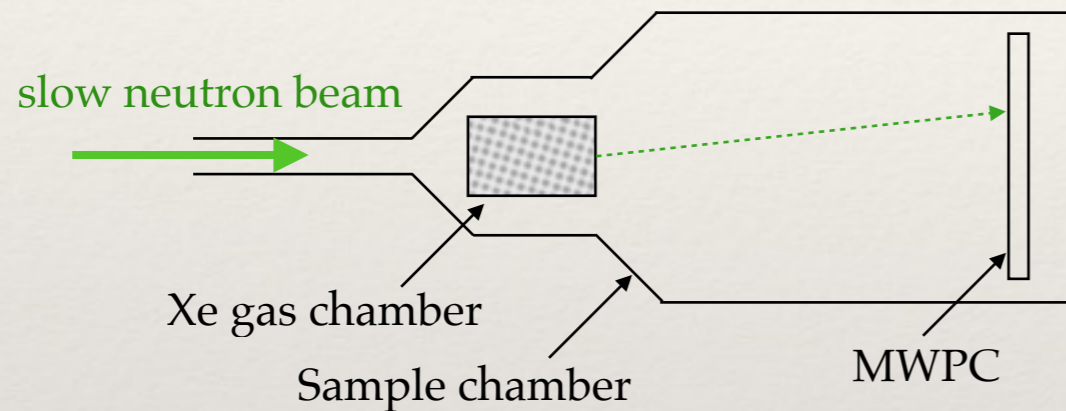
interaction range :  $\lambda \equiv \frac{1}{\mu}$



# 1.1 Current limits

- ❖  $\lambda < 10$  nm  
neutron scattering

- ❖ e.g. Kamiya et al. (2015)



- ❖ Precise measurement of scattering angle distribution
- ❖ Slow neutron beam ( $\lambda=5\text{\AA}$ ,  $E\sim 3\text{meV}$ )
- ❖ 2 atm Xenon

# 2. Scattering law



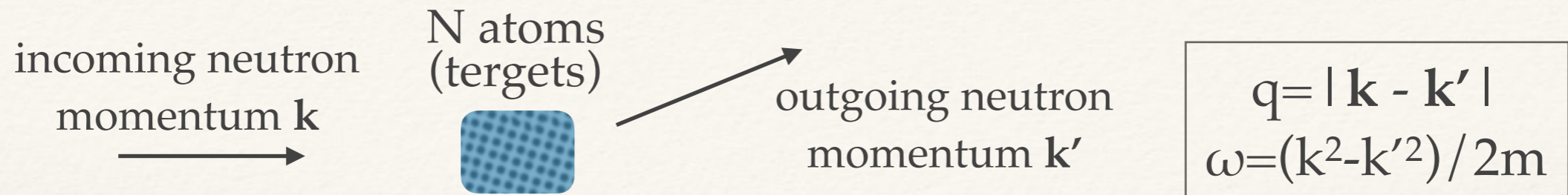
$$q = |\mathbf{k} - \mathbf{k}'|$$
$$\omega = (k^2 - k'^2) / 2m$$

❖ differential cross section :

coherent / incoherent scattering length

$$\frac{d^2\sigma}{d\Omega d\omega} = N \frac{k'}{k} [b_{\text{coh}}^2(q) S_c(q, \omega) + b_i^2 S_i(q, \omega)]$$

# 2. Scattering law



❖ differential cross section :

coherent / incoherent scattering length

$$\frac{d^2\sigma}{d\Omega d\omega} = N \frac{k'}{k} [b_{\text{coh}}^2(q) S_c(q, \omega) + b_i^2 S_i(q, \omega)]$$

dynamic structure factor

$$S_c(q, \omega; T, \rho) = \frac{1}{2\pi N} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_{j, j'} \langle e^{-i\mathbf{q} \cdot \mathbf{R}_j(0)} e^{i\mathbf{q} \cdot \mathbf{R}_{j'}(t)} \rangle$$

$$S_i(q, \omega; T, \rho) = \frac{1}{2\pi N} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_j \langle e^{-i\mathbf{q} \cdot \mathbf{R}_j(0)} e^{i\mathbf{q} \cdot \mathbf{R}_j(t)} \rangle$$

$j$  : indices of atoms

$\mathbf{R}_j$  : the position of  $j$  th atom

# 2. Scattering law



❖ differential cross section :

coherent / incoherent scattering length

$$\frac{d^2\sigma}{d\Omega d\omega} = N \frac{k'}{k} [b_{\text{coh}}^2(q) S_c(q, \omega) + b_i^2 S_i(q, \omega)]$$

dynamic structure factor

$$S_c(q, \omega; T, \rho) = \frac{1}{2\pi N} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_{j, j'} \langle e^{-i\mathbf{q} \cdot \mathbf{R}_j(0)} e^{i\mathbf{q} \cdot \mathbf{R}_{j'}(t)} \rangle$$

$$S_i(q, \omega; T, \rho) = \frac{1}{2\pi N} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_j \langle e^{-i\mathbf{q} \cdot \mathbf{R}_j(0)} e^{i\mathbf{q} \cdot \mathbf{R}_j(t)} \rangle$$

$j$  : indices of atoms

$\mathbf{R}_j$  : the position of  $j$  th atom

static structure factor

$$\frac{d\sigma}{d\Omega} = N \frac{k'}{k} [b_{\text{coh}}^2(q) S(q) + b_i^2]$$

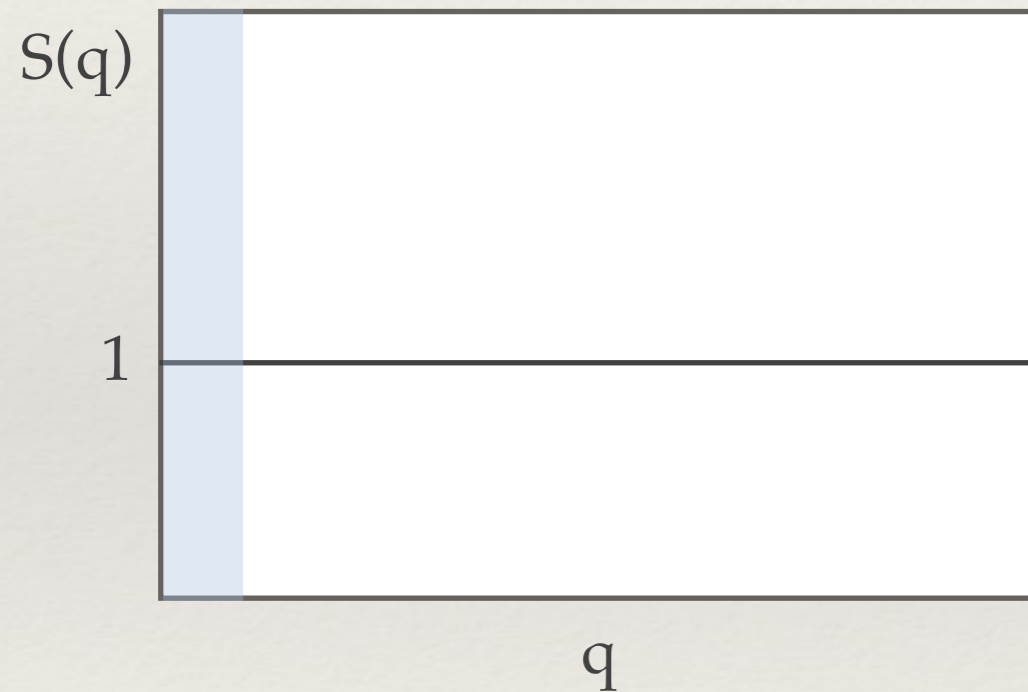
“sum rule”

$$S_0 \equiv S(0) = \rho \kappa_T k_B T = \left( \frac{\partial \rho}{\partial P} \right)_T k_B T$$

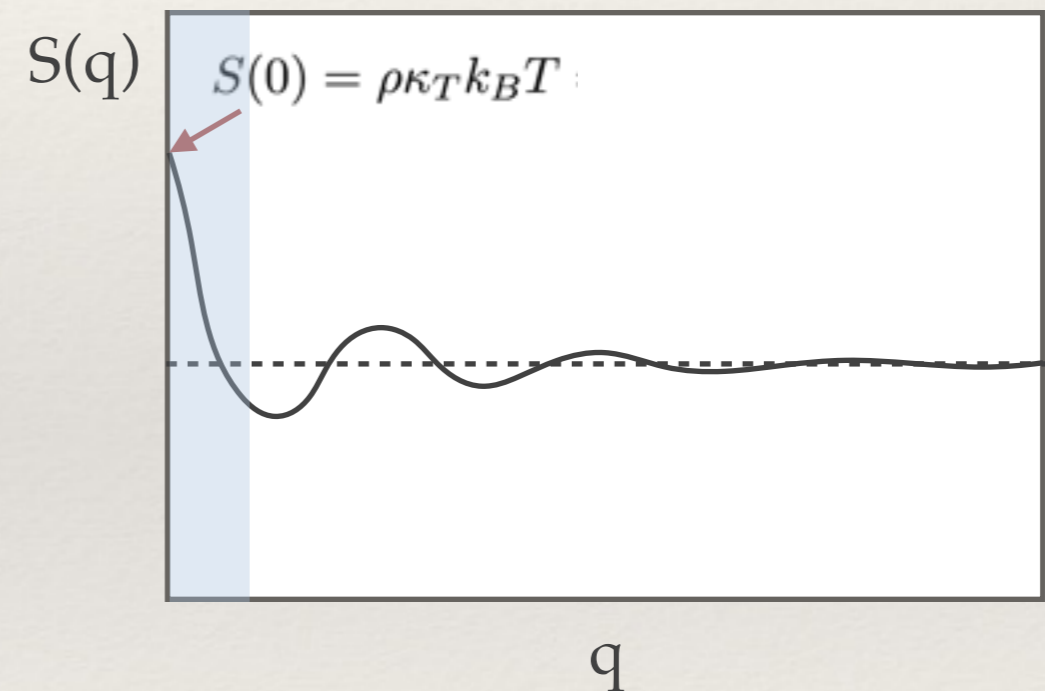
# 2. Scattering law

$$\frac{d\sigma}{d\Omega} = N \frac{k'}{k} [b_{\text{coh}}^2(q) S(q) + b_i^2]$$

for ideal gas (illustration)



for dense gas (illustration)





# 2.1 coherent scattering length

- ❖ General expression (leading term, for cold neutron) :

$$b_{\text{coh}}(q) \approx b_c - b_e Z [1 - f(q)]$$

$$b_c = b_{N_e} + b_{N_p}$$

the neutron electric polarization  
 the strong interaction

for Kr

~ 8.0 fm

$$b_e = b_F + b_I$$

intrinsic n-e scattering length  
 neutron charge distribution - electron

~  $-1.5 \times 10^{-3}$  fm

Foldy scattering length

neutron magnetic moment - charge density of atom

~  $-1.3 \times 10^{-3}$  fm

- ❖  $f(q)$  : the atomic form factor (the empirical form)

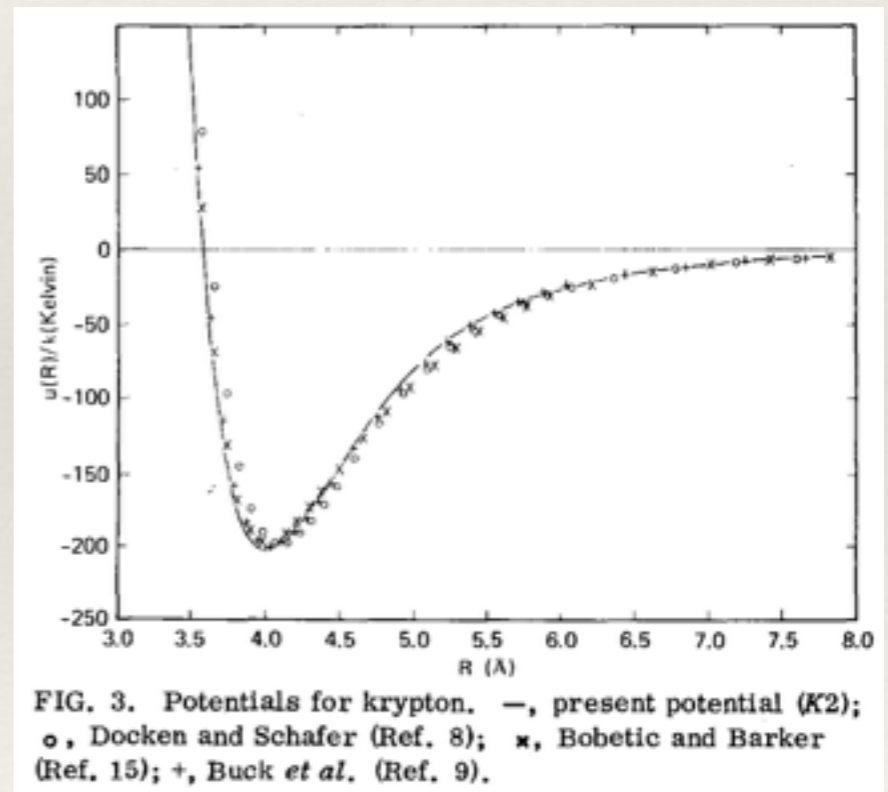
$$f(q) = \frac{1}{\sqrt{1 + 3(q/q_0)^2}} \quad q_0 = 1.9 Z^{1/3} [1/\text{\AA}]$$

# 2.2 static structure factor

- ❖ interatomic potential :  $\varphi(r) \propto r^{-6}$  ( $r \rightarrow \infty$ )  
...due to the van der Waals force

- ❖ According to the fluid structure theory :

$$\frac{1}{2\pi^2\rho r} \int_0^\infty dq \left\{ q \frac{S(q) - 1}{S(q)} \right\} \sin qr \sim -\beta\varphi(r) \propto r^{-6} \quad \text{as } r \rightarrow \infty$$



Barker et al. J. Chem. Phys., 61 (1974)

# 2.2 static structure factor

- ❖ interatomic potential :  $\varphi(r) \propto r^{-6}$  ( $r \rightarrow \infty$ )  
...due to the van der Waals force

- ❖ According to the fluid structure theory :

$$\frac{1}{2\pi^2 \rho r} \int_0^\infty dq \left\{ q \frac{S(q) - 1}{S(q)} \right\} \sin qr \sim -\beta \varphi(r) \propto r^{-6} \quad \text{as } r \rightarrow \infty$$

- ❖ From the results of “the asymptotic Fourier analysis”

$$\frac{1}{r} \int_0^\infty F(q) \sin qr dq \sim \frac{F(0)}{r^2} - \frac{F''(0)}{r^4} + \frac{F^{iv}(0)}{r^6} - \dots$$

$\downarrow$   
=0
 $\downarrow$   
=0

$$F(q) \equiv q \{1 - S^{-1}(q)\} \quad F''(0) = -\frac{2S'(0)}{S^2(0)} = 0 \Leftrightarrow S'(0) = 0$$

$$S(q) = S_0 + S_2 q^2 + S_3 q^3 + S_4 q^4 \dots$$

# 3. Scattering length with new interactions

- ❖ The potential due to new interactions :

$$V_{\text{new}}(r) = -\frac{1}{4\pi}g^2Q_1Q_2\frac{e^{-\mu r}}{r} \xrightarrow{\text{Born approx.}} b_{\text{new}}(q) = \frac{m_n}{2\pi}g^2Q_1Q_2\frac{1}{\mu^2 + q^2}$$

- ❖ The scattering length :

$$b_{\text{coh}}(q) \approx b_c - b_e Z[1 - f(q)] + b_{\text{new}}(q)$$

$$= b_c \left\{ 1 + \chi_{\text{em}}[1 - f(q)] + \chi_{\text{new}}\frac{\mu^2}{q^2 + \mu^2} \right\}$$

$$\chi_{\text{em}} \equiv -\frac{b_e}{b_c}Z \quad \chi_{\text{new}} \equiv \frac{m_n}{2\pi}g^2Q_1Q_2\frac{1}{b_c\mu^2}$$

For Kr,  $\chi_{\text{em}} \sim 10^{-2}$   $\chi_{\text{new}} \sim 10^{-3}$  ( $1/\mu = 10^{-9}m$ ,  $g^2 = 10^{-15}$ )

# 3. Scattering length with new interactions

- ❖ The potential due to new interactions :

$$V_{\text{new}}(r) = -\frac{1}{4\pi}g^2Q_1Q_2\frac{e^{-\mu r}}{r} \xrightarrow{\text{Born approx.}} b_{\text{new}}(q) = \frac{m_n}{2\pi}g^2Q_1Q_2\frac{1}{\mu^2 + q^2}$$

- ❖ The scattering length :

$$b_{\text{coh}}(q) \approx b_c - b_e Z[1 - f(q)] + b_{\text{new}}(q)$$

$$= b_c \left\{ 1 + \chi_{\text{em}}[1 - f(q)] + \chi_{\text{new}}\frac{\mu^2}{q^2 + \mu^2} \right\}$$

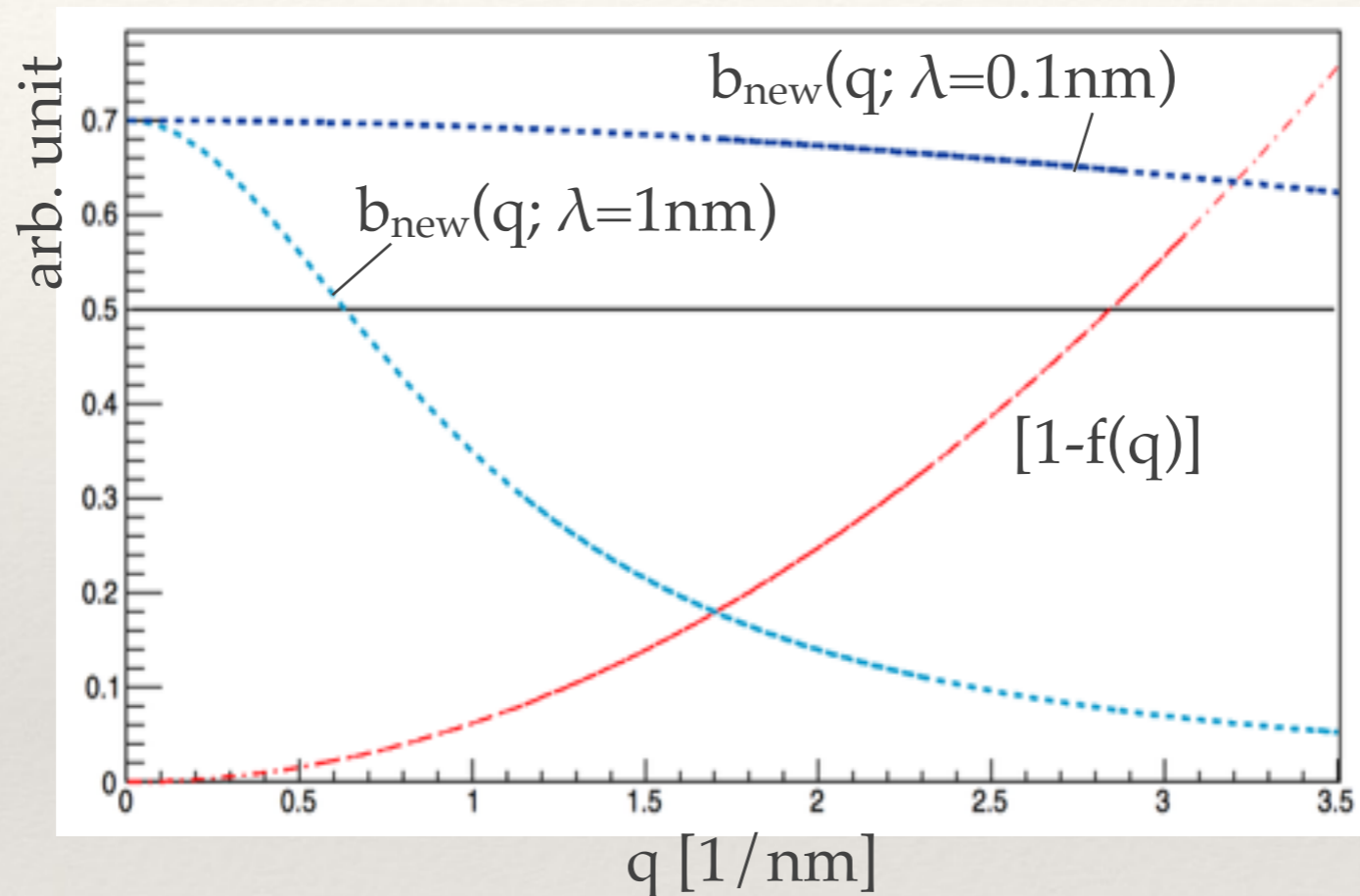
$$\chi_{\text{em}} \equiv -\frac{b_e}{b_c}Z \quad \chi_{\text{new}} \equiv \frac{m_n}{2\pi}g^2Q_1Q_2\frac{1}{b_c\mu^2}$$

For Kr,  $\chi_{\text{em}} \sim 10^{-2}$      $\chi_{\text{new}} \sim 10^{-3}$     ( $1/\mu = 10^{-9}m$ ,  $g^2 = 10^{-15}$ )

$$b_{\text{coh}}^2(q) \approx b_c^2 \left\{ 1 + 2\chi_{\text{em}}[1 - f(q)] + 2\chi_{\text{new}}\frac{\mu^2}{q^2 + \mu^2} \right\}$$

# 3. Scattering length with new interactions

$$b_{\text{coh}}^2(q) \approx b_c^2 \left\{ 1 + 2\chi_{\text{em}}[1 - f(q)] + 2\chi_{\text{new}} \frac{\mu^2}{q^2 + \mu^2} \right\}$$

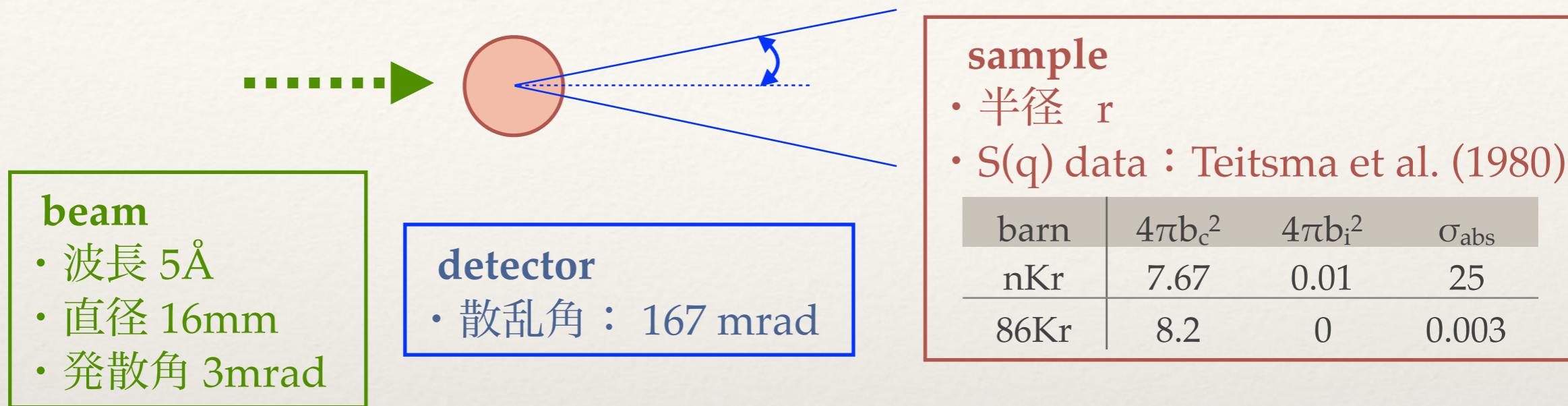


The differential cross section (coherent term) :

$$\begin{aligned} \left( \frac{d\sigma}{d\Omega} \right)_{\text{coh}} &= N \frac{k'}{k} b_c^2(q) S(q) \\ &= N \frac{k'}{k} \times b_c^2 \left\{ 1 + 2\chi_{\text{em}}[1 - f(q)] + 2\chi_{\text{new}} \frac{\mu^2}{q^2 + \mu^2} \right\} \times (S_0 + S_2 q^2 + S_3 q^3 + \dots) \end{aligned}$$

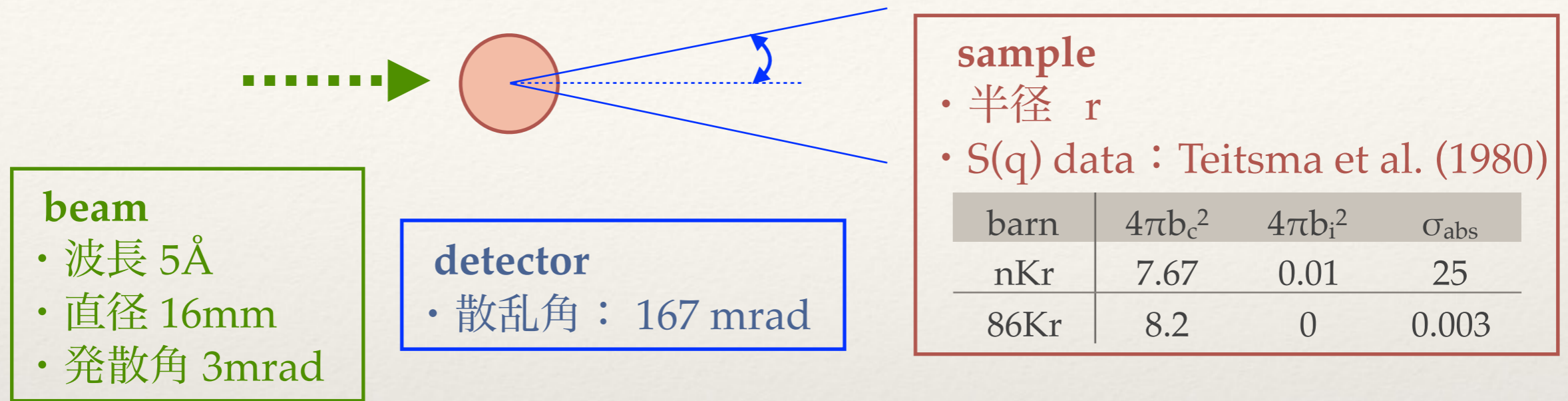
# 4. 実験条件の検討

❖ シミュレーション(with McStas)のセットアップ



# 4. 実験条件の検討

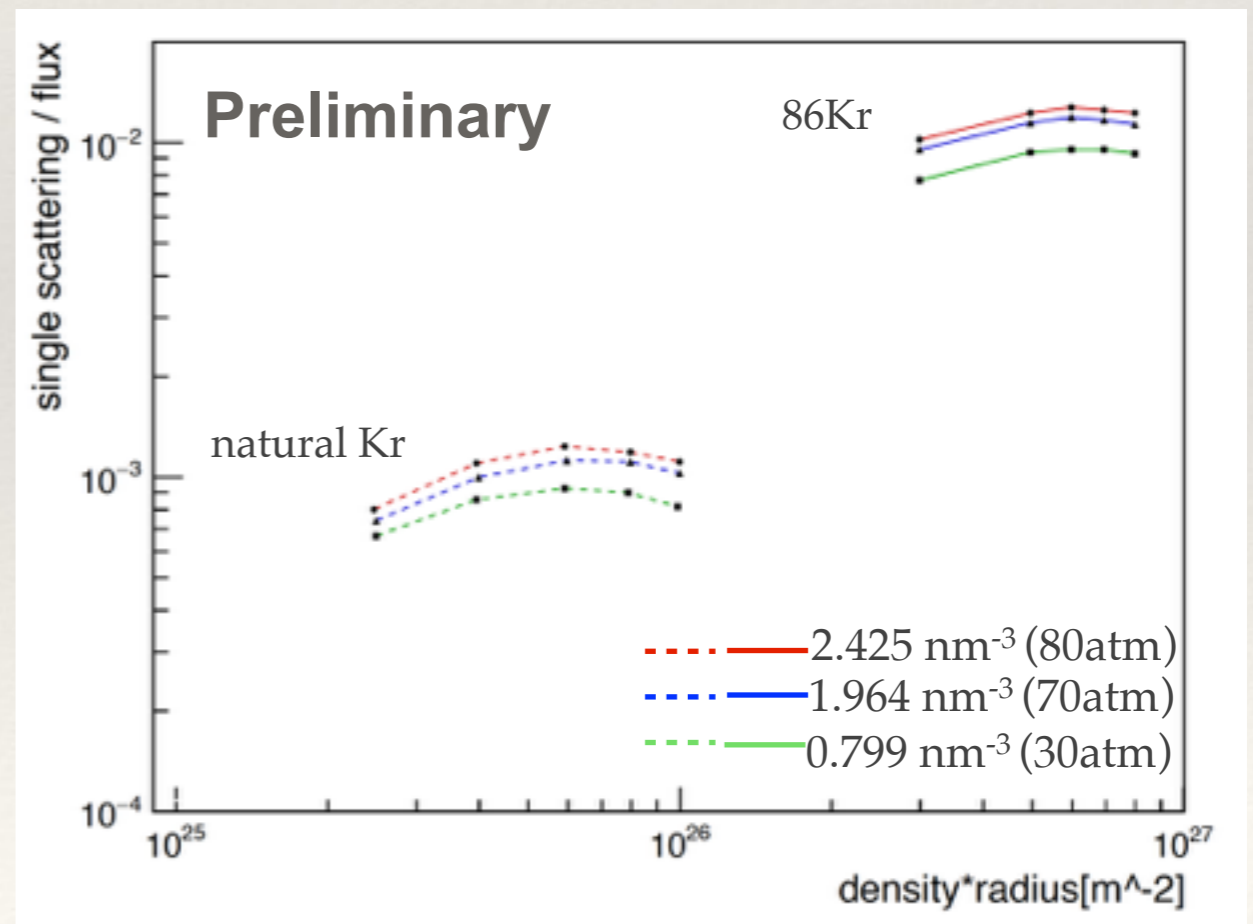
❖ シミュレーション(with McStas)セットアップ



❖ 自己遮蔽により散乱強度は頭打ち

❖ 最も強くなる条件

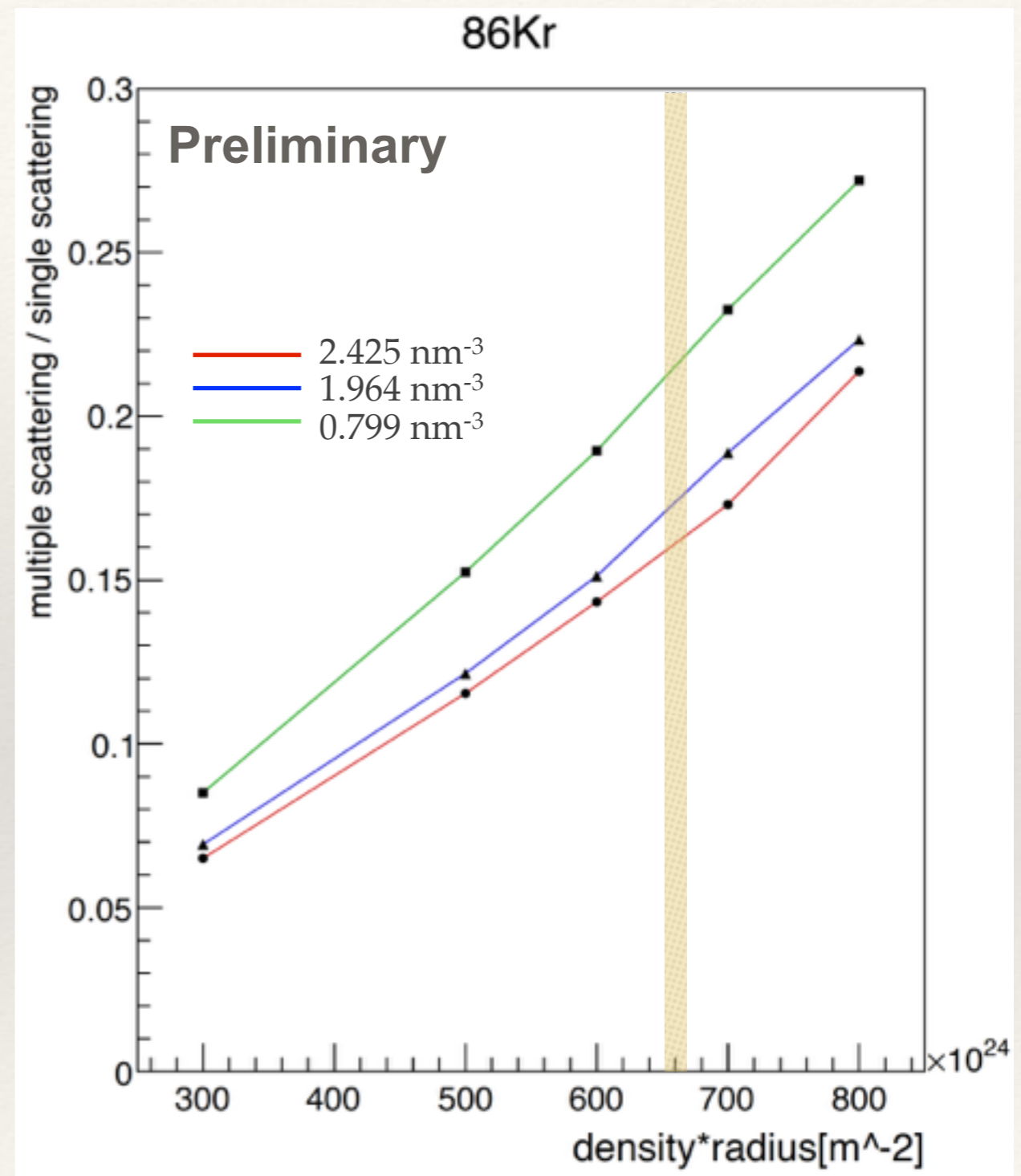
	density*radius[m <sup>-2</sup> ]
nKr	$6.2 \times 10^{25}$
86Kr	$6.6 \times 10^{26}$





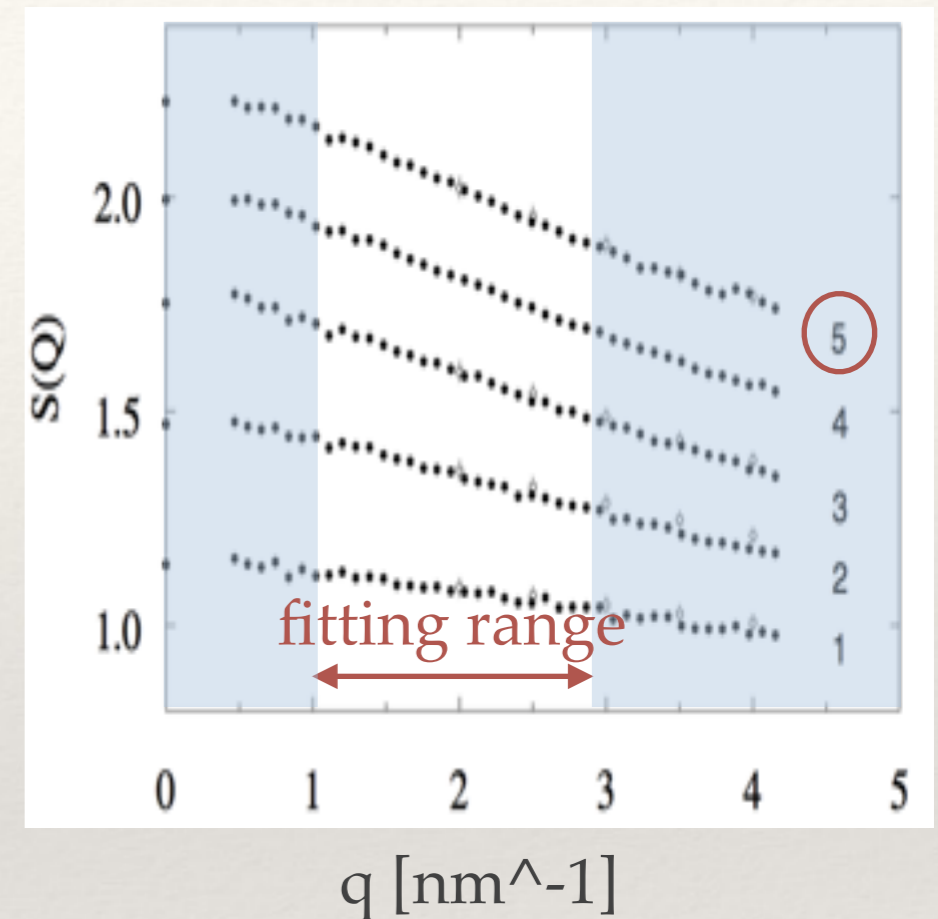
# 4. 実験条件の検討

- ❖ 1回散乱と多重散乱の比
- ❖ 86Krの1回散乱が最大  
→ 多重散乱 > 10%
- ❖ 仮に多重散乱 < 1%未満  
とすると 86Krにするご利益はない



# 5. Analysis

- ❖ Benmore et al. J. Phys.: Condens. Matter, **11**, 3091(1999)
- ❖ Experimental conditions
  - ❖ **86Kr** gas fluid,  $\sigma_c = 4\pi b_c^2 = 8.2 \pm 0.5$  [barn]
  - ❖  $T = 297.6 \pm 0.5$  K
  - ❖  $\rho = 0.804, 1.522, 1.984, 2.231, \underline{2.431} \text{ nm}^{-3}$  ( $\sim 80 \text{ atm}$ )
  - ❖ the statistical error : 0.5%



# 5. Analysis

❖ Benmore et al. J. Phys.: Condens. Matter, **11**, 3091(1999)

❖ Experimental conditions

❖ **86Kr** gas fluid,  $\sigma_c = 4\pi b_c^2 = 8.2 \pm 0.5$  [barn]

❖  $T = 297.6 \pm 0.5$  K

❖  $q = 0.804, 1.522, 1.984, 2.231, \underline{2.431 \text{ nm}^{-3}} (\sim 80 \text{ atm})$

❖ the statistical error : 0.5%

❖ The fitting function

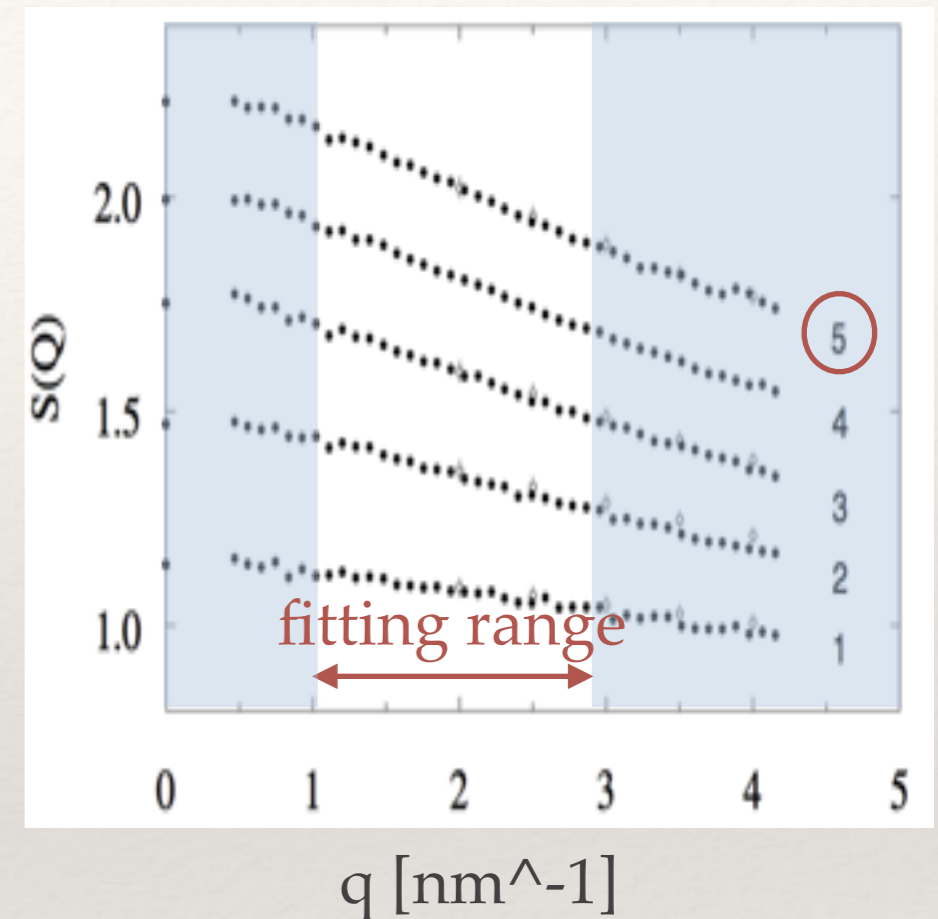
$$\left\{ 1 + 2\chi_{\text{em}}[1 - f(q)] + 2\chi_{\text{new}} \frac{\mu^2}{q^2 + \mu^2} \right\} \times (S_0 + S_2 q^2 + S_3 q^3)$$

$$S_0 = 1.423 \pm 0.008$$

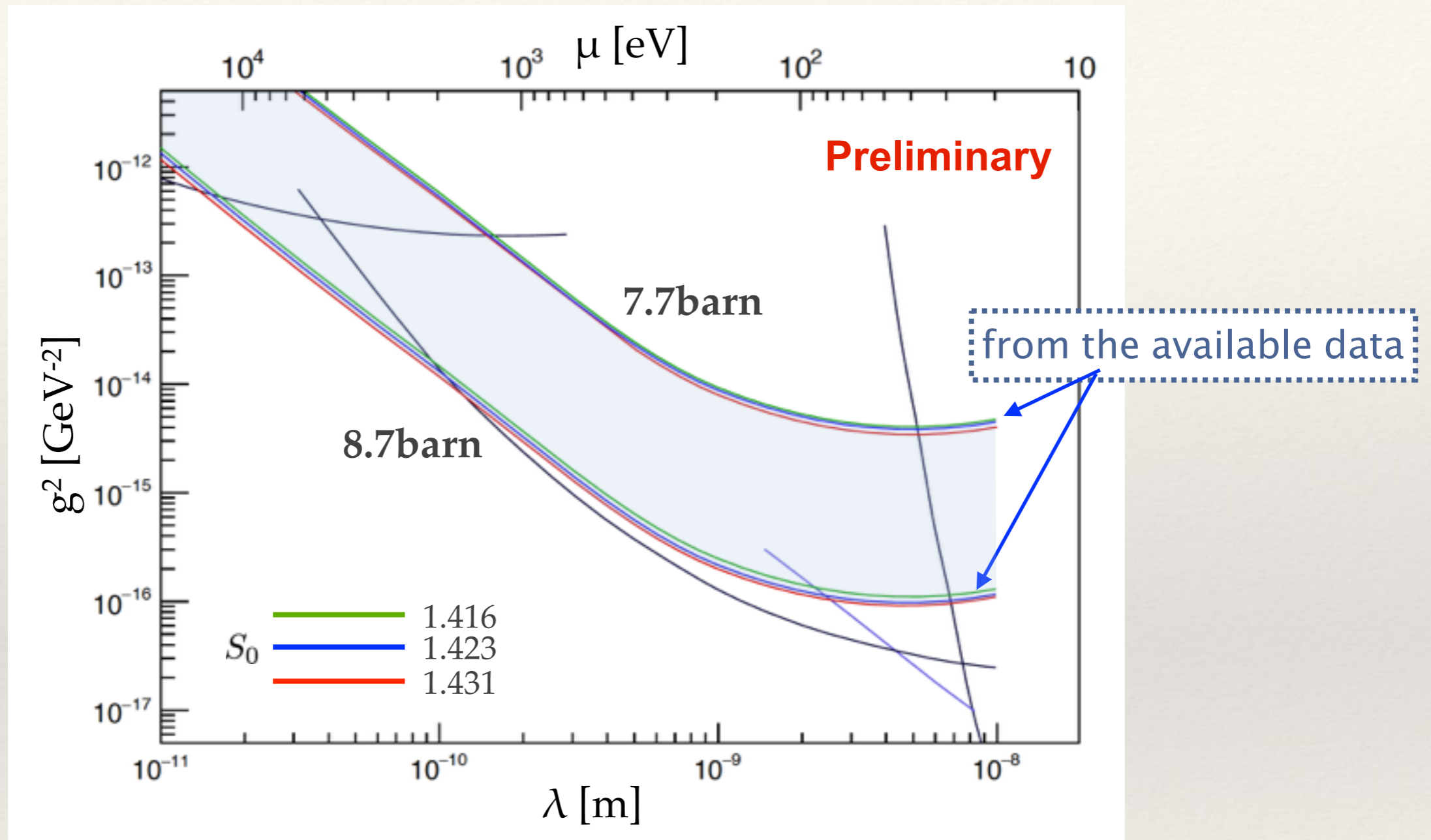
❖ The fitting range :  $1 < q < 2.8 \text{ nm}^{-1}$

❖ lower limit : to ignore the retardation effect

❖ upper limit : to avoid contributions of higher order terms



# 5. Analysis



---

# 6. Summary

---

- ❖ 濃縮流体を用いた、質量に結合する未知短距離力の探索手法を開発
- ❖ natural Kr,  $^{86}\text{Kr}$ サンプルに対する散乱強度および多重散乱を評価
  - ❖  $^{86}\text{Kr}$ を用いるメリットは無い(多重散乱/1回散乱 $<1\%$ )
- ❖  $^{86}\text{Kr}$ 小角散乱実験のデータに本手法を適用
  - ❖ 断面積の不定性、 $S_0$ の不定性を考慮し、到達感度を評価

今後

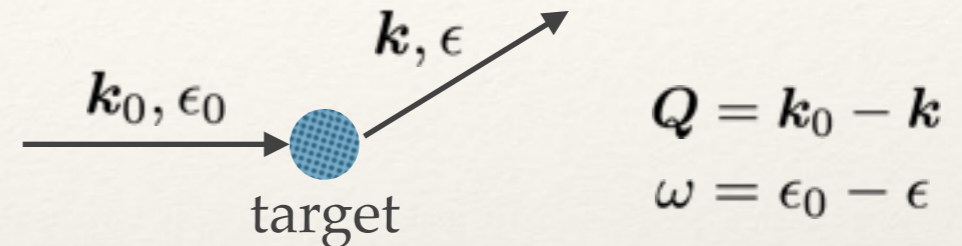
- ❖ 他の不定性(純度, 温度変化, 散乱位置等)を考慮し解析

# Multiple Scattering

- ❖ The Double Differential Cross Section **in the small-sample limit**

$$\frac{d^2\sigma}{d\Omega d\epsilon} = N \frac{\sigma_s}{4\pi} \frac{k}{k_0} S(Q, \omega)$$

- ❖  $N$  : the number of target atoms
- ❖  $\sigma_s$  : the scattering cross section
- ❖  $S(Q, \omega)$  : the dynamical structure factor (the Van Hove response func.)



- ❖ The Double Differential Cross Section (the general form)

$$\frac{d^2\sigma}{d\Omega d\epsilon} = N \frac{\sigma_s}{4\pi} \frac{k}{k_0} \sum_{j=0}^{\infty} s_j(\mathbf{k}_0, \mathbf{k})$$

- ❖  $s_j(\mathbf{k}_0, \mathbf{k})$  : the contribution from neutrons which have been scattered  $j$  times
  - ❖ single  $s_1(\mathbf{k}_0, \mathbf{k}) = S(\mathbf{Q}, \omega) H_1(\mathbf{k}_0, \mathbf{k})$
  - ❖ double  $s_2(\mathbf{k}_0, \mathbf{k}) = \frac{n\sigma_s}{4\pi} \int d\Omega_1 d\epsilon_1 S(\mathbf{Q}_1, \omega_1) S(\mathbf{Q}_2, \omega_2) H_2(\mathbf{k}_0, \mathbf{k}_1, \mathbf{k})$
  - ...

\*  $H_j(\mathbf{k}_0, \dots, \mathbf{k})$ : the transmission factor

- We require a knowledge of  $S(Q, \omega)$   
 → multiple scat. corrections are important

